SAMRAI

Center for Applied Scientific Computing

Structured Adaptive Mesh Refinement Application Infrastructure

SAMRAI is an object-oriented software framework for structured adaptive mesh refinement (SAMR) research. SAMRAI provides computational scientists with flexible support for exploring new parallel structured AMR applications. The primary goal of the SAMRAI effort is to facilitate the development of SAMR applications that require complex coupled physics models, sophisticated solution methods, and high-performance parallel computing hardware.

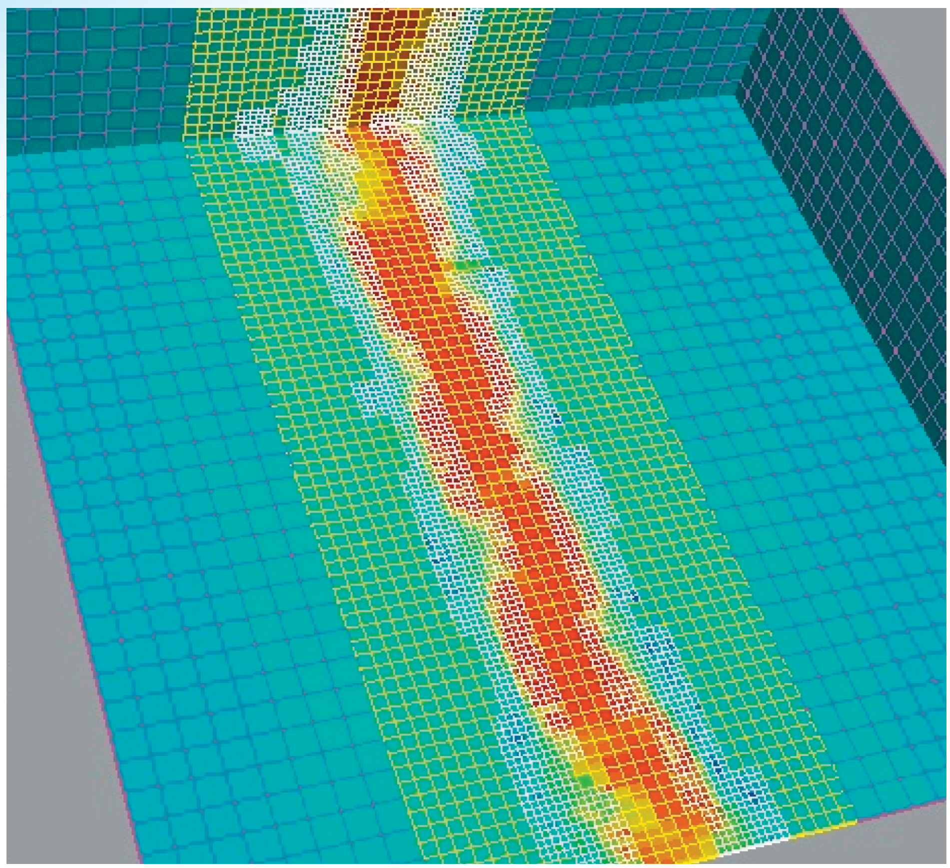

Figure 1. In this hybrid continuum-particle simulation, SAMR concentrates particles to resolve mixing of two gasses. Particles exist only in the finest cells (white boundaries).

Background

Advances in high-performance computing hardware enable the simulation of large three-dimensional problems that involve complex chemical and physical processes. In many important science and engineering applications, salient features of the simulation occur in localized regions of the computational domain.

Employing a uniform computational mesh to resolve local phenomena can be an inefficient use of computational resources. Structured adaptive mesh refinement (SAMR) provides a systematic way to focus CPU time and memory resources by applying varying degrees of local spatial and temporal resolution (Figure 1). Thus, SAMR is an important technology for the development of large-scale, three-dimensional simulations with complex physics.

Emerging SAMR Application Domains

The SAMRAI team and its collaborators are investigating the application of SAMR technology to new application domains. SAMRAI collaborations include projects at the Lawrence Livermore National Laboratory (LLNL) and universities such as The Utah ASCI Alliance Center. (ASCI is the Advanced Simulation and Computing, a national effort to develop reliable terascale computing.) Our laboratory collaborations involve simulation of laser–plasma instabilities, Richtmyer–Meshkov multi-fluid interface instabilities, and the combination of AMR with ALE hydrodynamics methods. The Utah ASCI Center is developing an integrated simulation code to model the effects of fire on containers of high explosives. These efforts emphasize large-scale parallelism, sophisticated linear and nonlinear solvers, coupled physics packages, hybrid integration methods that combine continuum and discrete representations, and complex data structures on SAMR meshes.

The application of SAMR to such problems gives rise to many interesting algorithmic, numerical, and computer science research questions. These issues are related to mathematical model approximations in a SAMR setting, dynamically adaptive integration methods, load balancing for distributed memory parallel computing, and object-oriented software framework design and development.

The SAMRAI Framework

The goals of SAMRAI are to:

- Support SAMR application development while reducing the need for expertise in parallel programming and SAMR infrastructure.
- Enable computational scientists to explore new applications and algorithms through the composition and extension of existing software components.

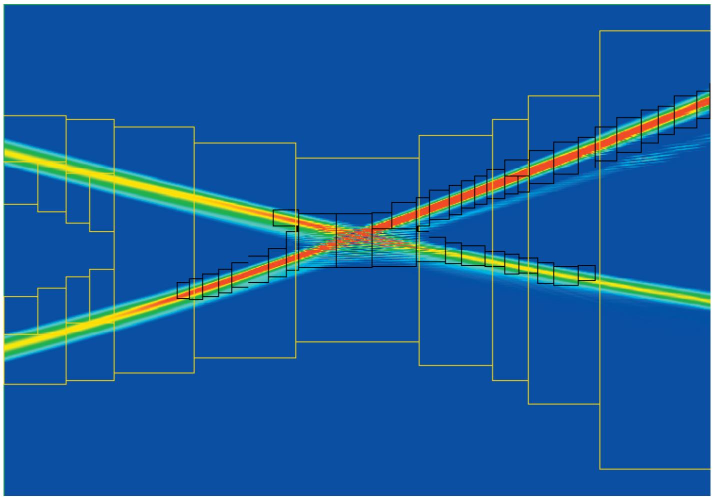

Figure 2. Locally refined grids resolve wave interaction of crossing beams in this laser–plasma simulation. Fine grids are placed around regions of high light intensity.

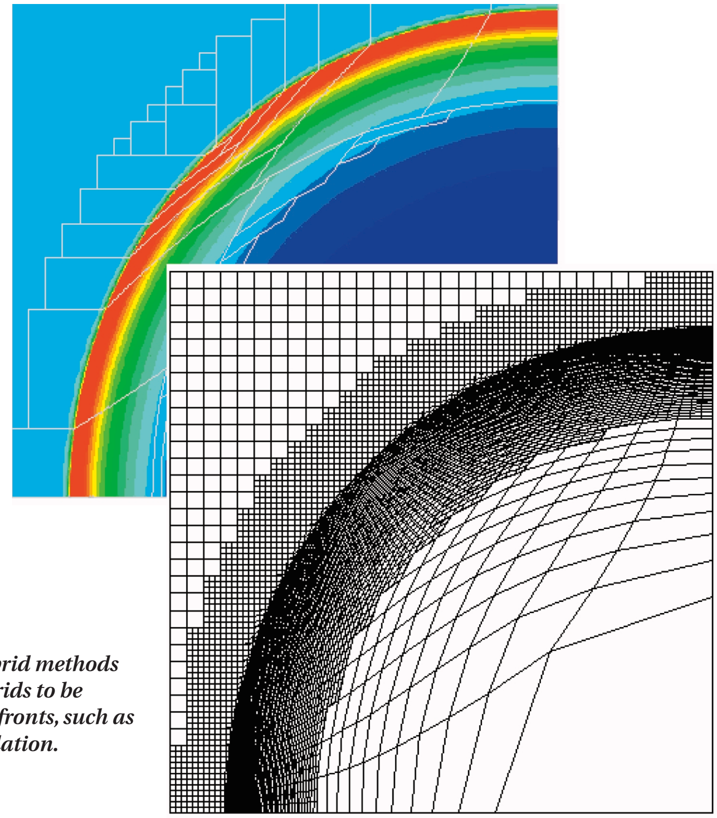

Figure 3. ALE–AMR hybrid methods allow refined moving grids to be placed around moving fronts, such as in this blast wave simulation.

- Reduce development time for new SAMR applications by leveraging existing software and solver technology.

Application scientists view SAMRAI as a collection of software packages tools from which to build an application. Many software components can be re-used across a broad spectrum of applications. Examples of common components include linear and nonlinear solvers, grid generators, parallel communication routines, variable management, data structures, time integration algorithms, and parallel data decomposition and mapping algorithms. In SAMRAI, these common components are factored into a single general-purpose toolbox from which complex applications are built.

We employ object-oriented design techniques that allow components to be enhanced without changing the underlying framework source code or re-compiling the library. For example, application developers may introduce new data types such as particles for discrete methods without modifying existing parallel communication routines, data structures, or algorithm support. We also address interoperability issues so that SAMRAI users may employ other software packages (such as linear and nonlinear solver libraries, including PETSc, KINSOL, and *hypre*) with SAMRAI.

SAMRAI Applications

SAMRAI is used in a variety of application development efforts in academia and LLNL. SAMRAI capabilities are validated and improved via these collaborations. New capabilities needed by an application are often integrated into the SAMRAI framework for use in other problems.

The ALPS (Adaptive Laser–Plasma Simulator) project at LLNL is investigating SAMR for use in the simulation of laser–plasma interaction (Figure 2). This is a critical process in understanding laser-driven fusion experiments. This application integrates three physics models: plasma hydrodynamics; a nonlinear potential equation; and laser light propagation. The entire algorithmic structure for explicit hydrodynamics developed for an earlier SAMRAI application was re-used without modification.

We are also collaborating with scientists at San Jose State and MIT to model Richtmyer–Meshkov instabilities using a hybrid approach that combines a continuum fluid description with a Discrete Simulation Monte Carlo (DSMC) particle representation at the interface (Figure 1). Both applications require complex data structures on SAMR grids, new integration algorithms, non-uniform load balancing, and sophisticated parallel communication techniques.

Another important effort at LLNL uses SAMRAI to investigate the combination of ALE methods used in ASCI codes with SAMR techniques for the simulation of shock hydrodynamics problems on high-performance parallel computers (Figure 3). The combination of ALE and SAMR may enable more highly resolved calculations than are reasonable with current ALE technology, such as detonation fronts with detailed chemistry.

For additional information about the SAMRAI project, visit our web site at http://www.llnl.gov/CASC/SAMRAI or contact: Richard Hornung, (925) 422-5097, hornung@llnl.gov.

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